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First Principles Modeling of Powder Absorption in Additive Manufacturing

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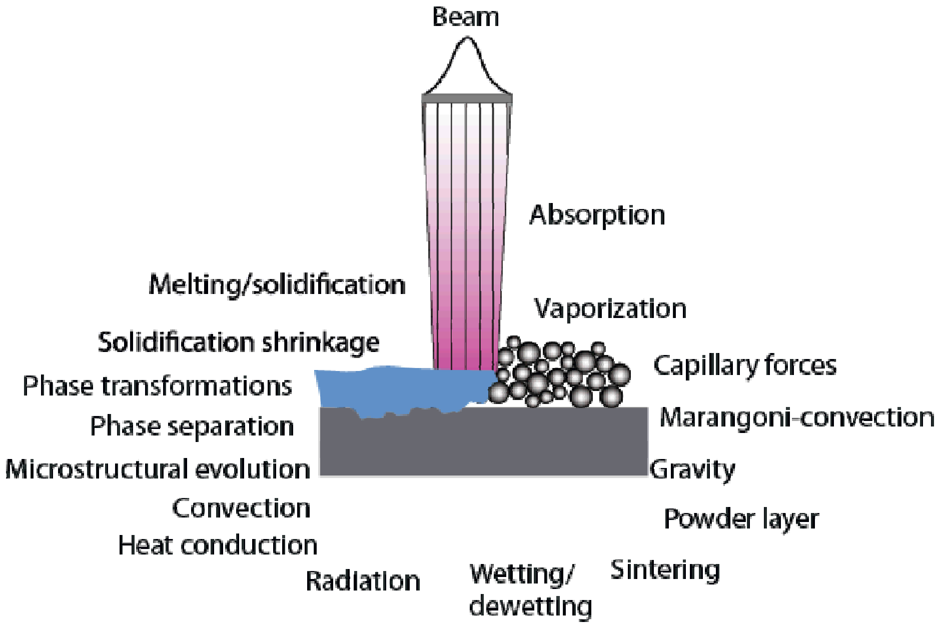
Laser radiation absorption is an important part of the complex physics of additive manufacturing process

Needed:

- Adequate absorption description is required for comprehensive process modeling.
- Models of effective media are not applicable.

Approach:

- We have used ray tracing, taking into account multiple Fresnel reflections/absorptions



This is the first 1st-principles 3D powder absorptivity simulation

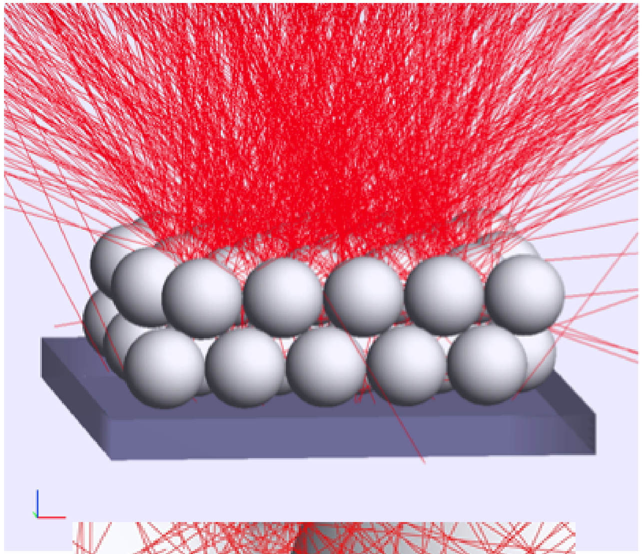
First principles calculations are being used to understand the absorptivity of the metal powder

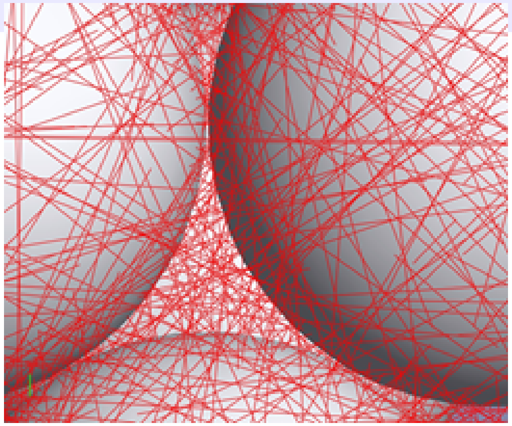
Needed:

- Calculate the absorptivity for selected materials, powder size distributions, and thicknesses

Approach:

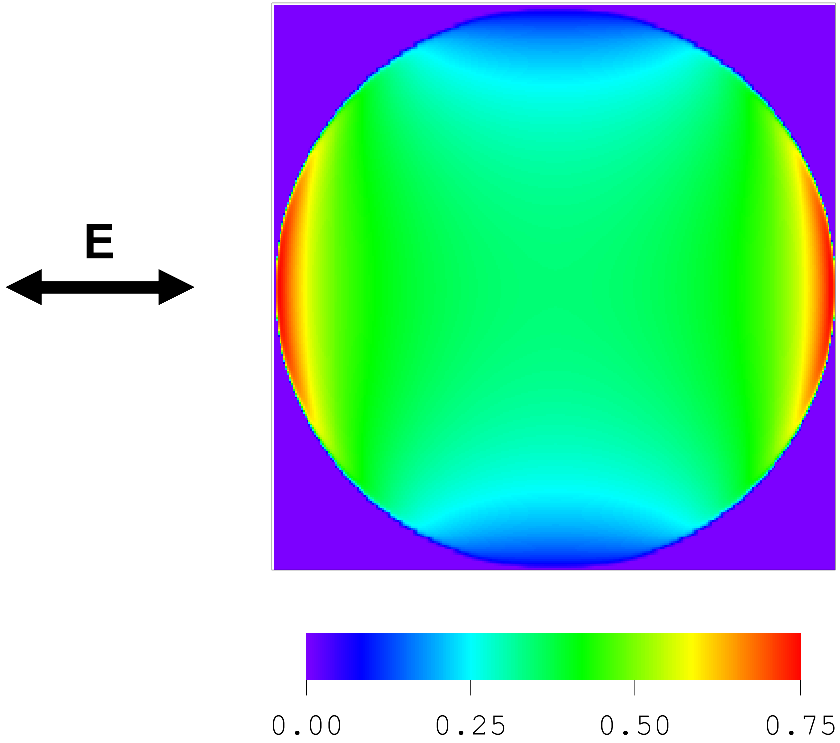
- Measure the refractive index as a function of temperature, in order to calculate the temperature dependence of the absorptivity (before melting starts)
- Evaluate the fluctuations of absorptivity due to the size distribution of the powder spheres, powder thickness and beam size





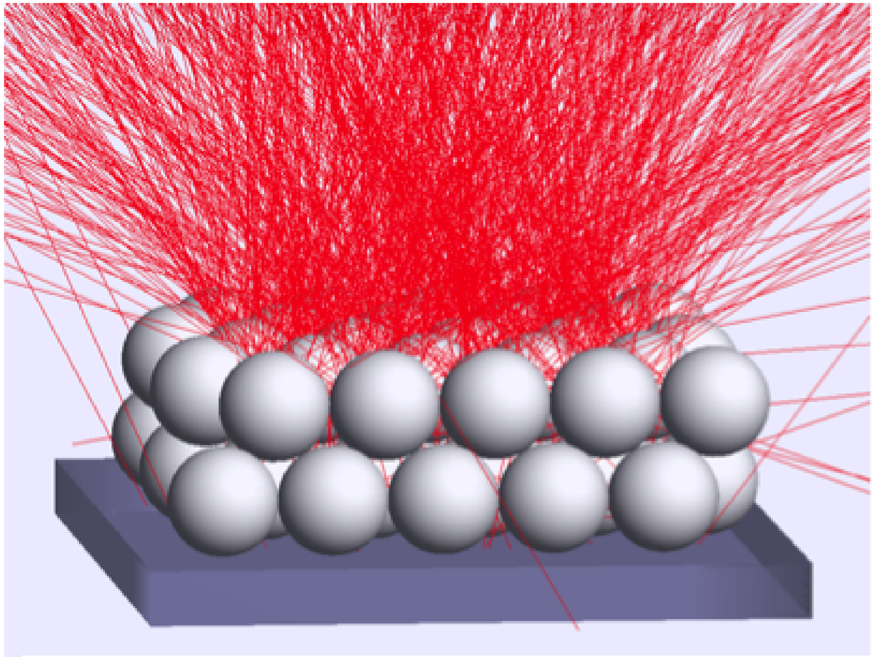
For a single sphere, the local absorptivity is a strong function of the incidence angle and polarization

Absorption distribution for a plane 1µm wave incident on a stainless steel sphere, *n* = 3.27 + 4.48 *i*



Dense packed powder with spheres of uniform size

- **Powder size (typically tens of microns) is much larger than the laser wavelength (1 μm), so ray tracing can be used**
- **The refractive index of the metals involved is known or can be measured**
- **On each reflection, the absorption is determined by Fresnel formulas, which include angular and polarization effects**
- **Multiple scattering plays an important role**
- **Commercial code FRED was used for ray tracing. Considerable post-processing was required.**



Stainless steel

Power balance

• Absorbed by top layer:	52%
• Absorbed by bottom layer:	6%
• Absorbed by substrate:	2%
• Reflected:	40%

Raytracing was performed via FRED software for optical systems

- FRED is developed and distributed by Photon Engineering (Tucson)
  - 3D graphical interface, along with script capability
  - Detailed source construction
  - Rays have position/direction, wavelength, polarization, power; both nonsequential and sequential raytracing
  - Numerous lenses, mirrors, prisms, vendor catalogs; interfaces with Code V, Zemax, and other optics codes

- How FRED was used here:
  - Source is assembly of incoherent laser rays incident on material
  - Material is assembly of thousands of metal spheres on substrate
    - Separate packaging program was used to generate spheres
    - Spheres were read into FRED and generated via script
  - Rays travel from surface to surface, with Fresnel absorption/reflection
  - Absorption in individual spheres is calculated via script

Modeling of powder absorption for selected metals

- Two layers of dense-packed metal spheres
- Uniform beam

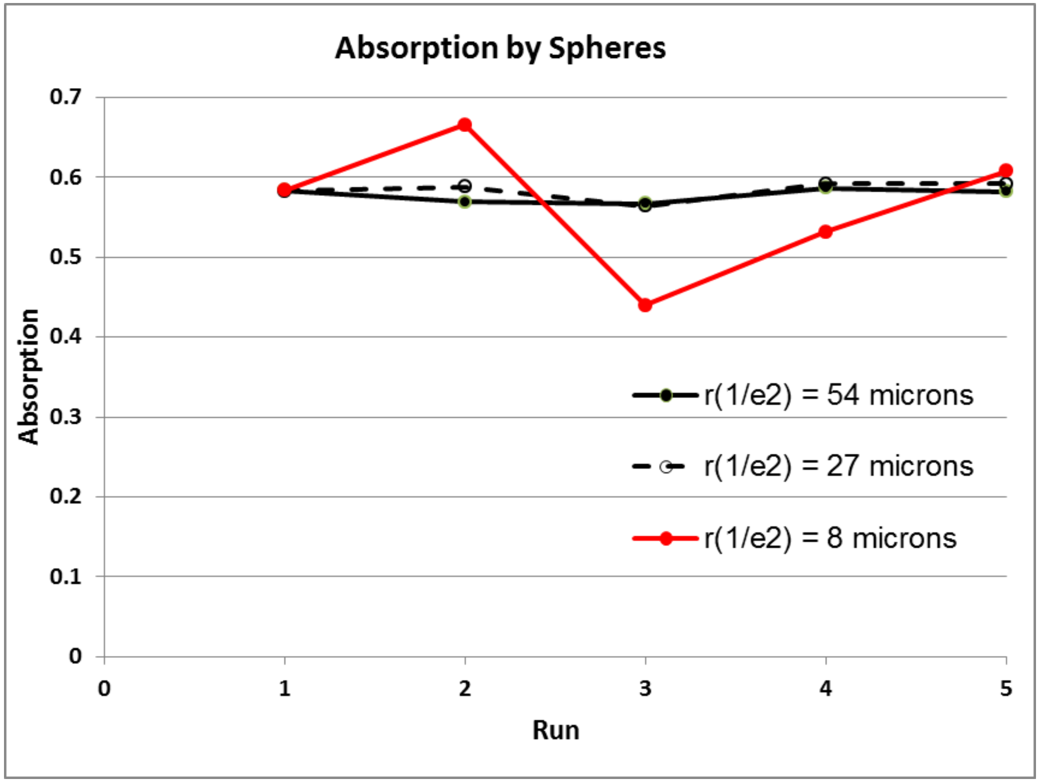
(1) Material	(2) Re(n)	(3) Im(n)	(4) α (flat surface)	(5) α (1 sphere)	(6) α (top layer)	(7) α (bottom layer)	(8) α (substrate)	(9) α (top + bottom)
Ag	0.23	7.09	0.018	0.020	0.070	0.042	0.008	0.11
Al	1.244	10.	0.047	0.056	0.151	0.061	0.011	0.21
Cu	0.35	6.97	0.028	0.032	0.098	0.050	0.009	0.15
SS	3.27	4.48	0.34	0.36	0.52	0.065	0.015	0.59
Ti	3.45	4.	0.38	0.40	0.56	0.065	0.016	0.62

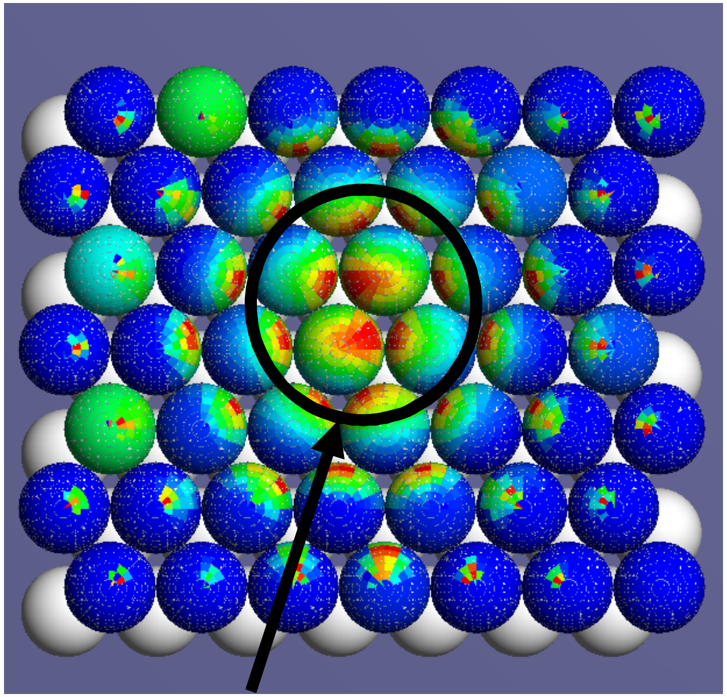
- Powder absorptivity is noticeably higher than the absorptivity of a flat surface or a single sphere

- The enhancement is more pronounced for highly reflective metals

If beam size is comparable with sphere diameter, overall absorption varies with beam position

- As a result, absorption width can exceed beam width
- Multiple scattering is important

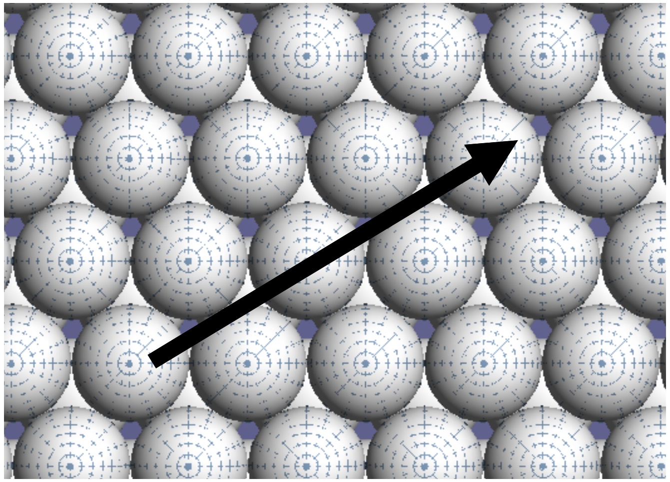




$1/e^2$ diameter Gaussian beam

Power deposition for scanning beam

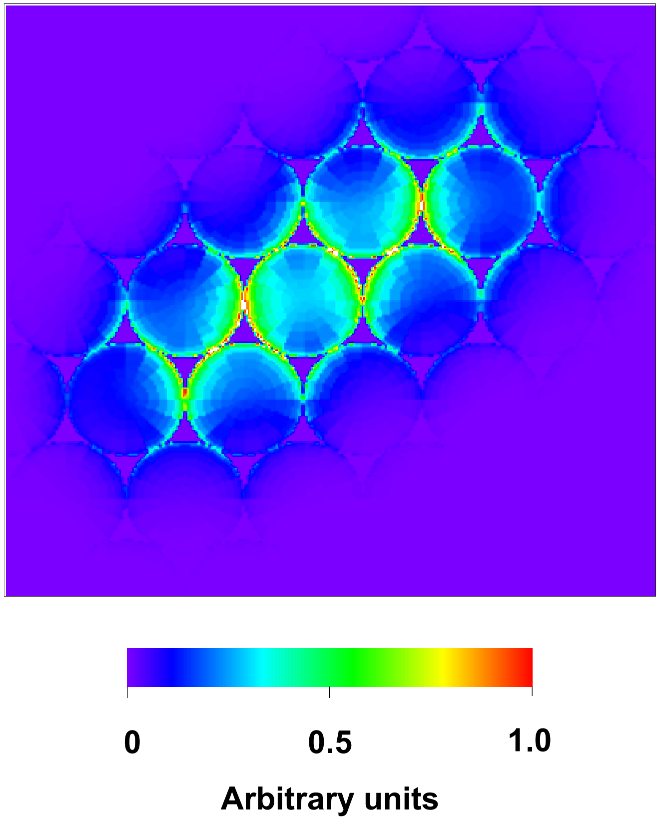
Path of beam center



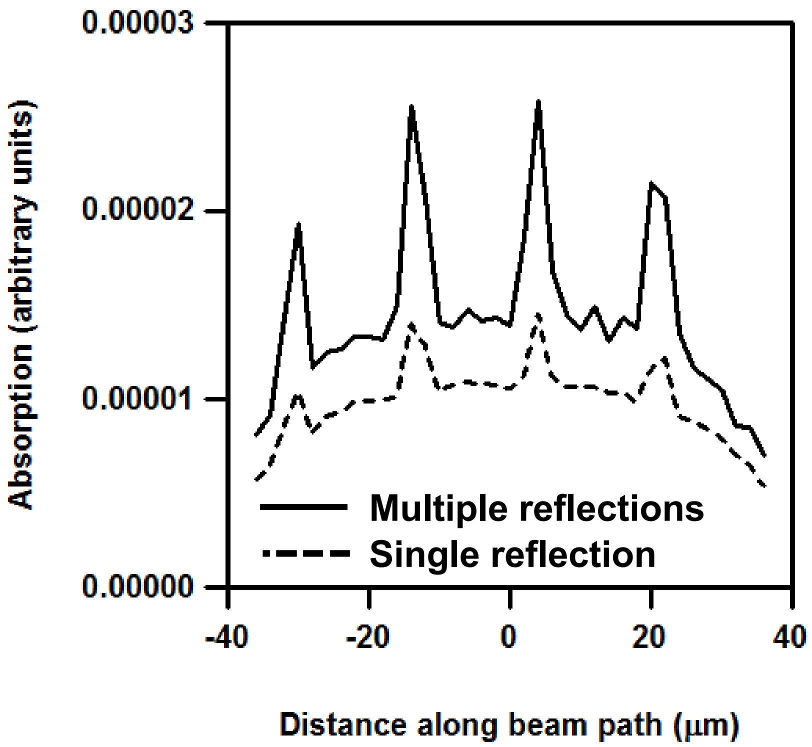
Overlapping beam imprints were recorded along arrow.

Distance between imprints: 20% sphere radius

Absorption



Absorption distribution in powder is highly non-uniform along the beam path



- Variations of absorption along the scan path are about 70% on the scale of the sphere radius
- Localization of absorption affects melt dynamics

We calculated the powder absorptivity for two realistic situations

(1) **We modeled the stainless steel powder used in Concept Laser system**

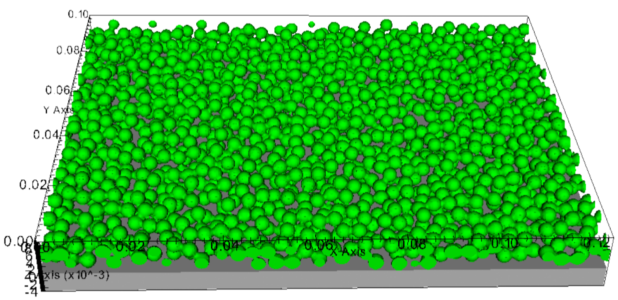
- **Gaussian distribution of particles with average size 27 μm and powder bed layer thickness 50 μm**
- **Beam size: D4σ-52μm**

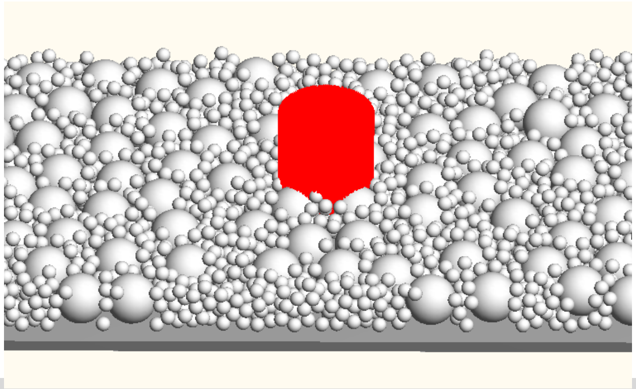
(2) **We used a bimodel powder that provided the maximal material density [1]**

- **Particle size ratio 1:7, with 20% volume of small spheres**

In each case, the powder pack algorithm of ALE3D was used to generate powder layers

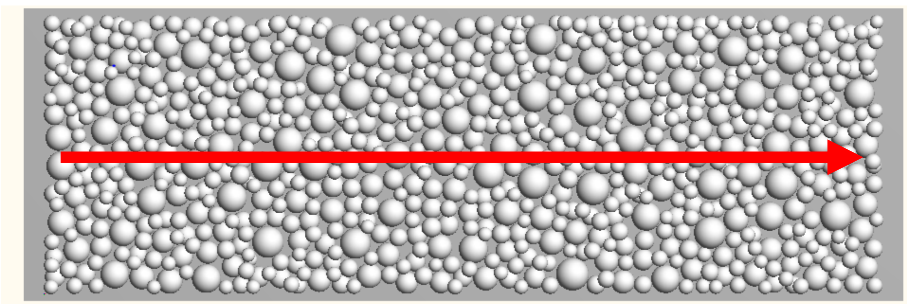
[1] R. Kelkar et al. "DMLM : Effect of bi-modal particle size distribution on surface finish," (2014)

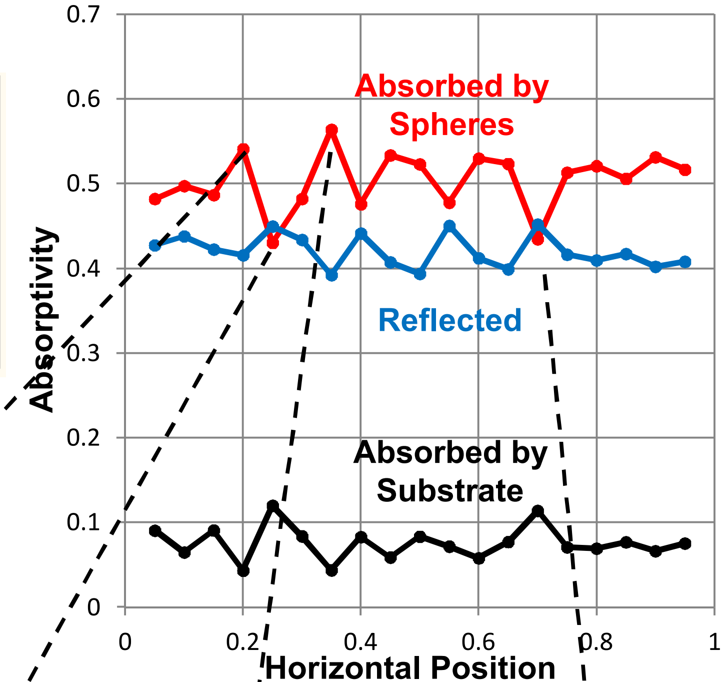




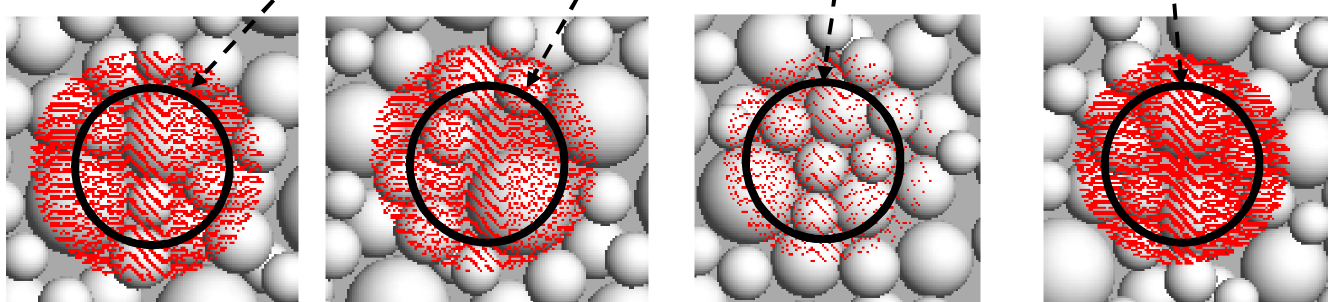
Absorptivity for several beam positions – Gaussian powder

- **Beam absorptivity was calculated along center strip**





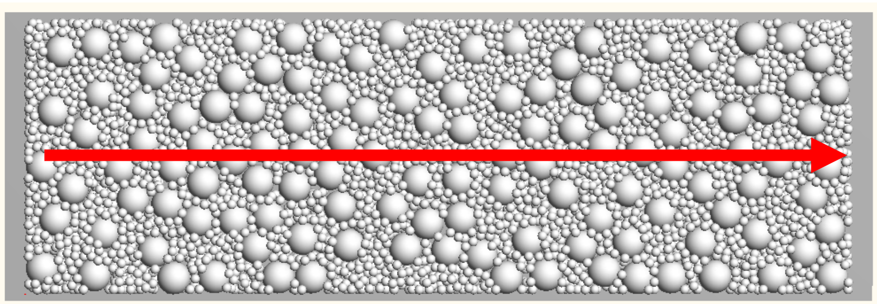
- **Maximum absorption by spheres occurs when beam fails to strike "hole" in powder**
- **Minimum absorption by spheres occurs when hole allows beam to reach substrate**



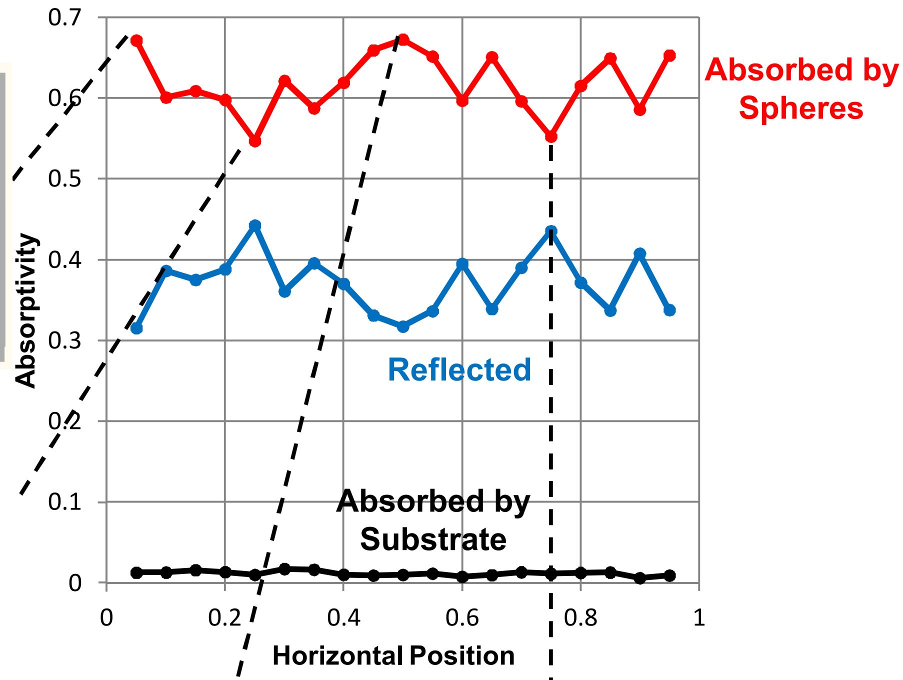
DoubledHalfMaxWidth_powder43microns_thick.txt

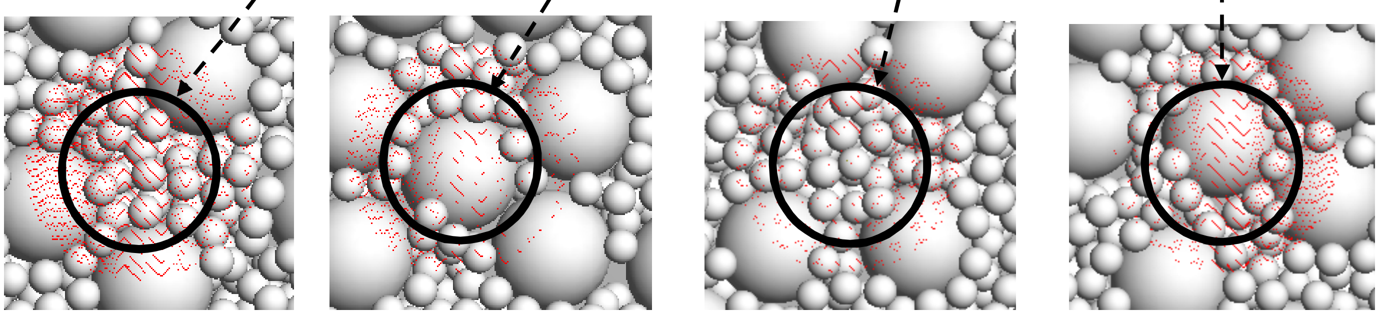
Absorptivity for several beam positions – bimodal powder

- **Beam absorptivity was calculated along center strip**



- **Maximum absorption occurs when beam strikes region of small spheres**
- **Minimum absorption occurs when beam is centered on a large sphere**





Absorption non-uniformity is important for melt evolution

- Time for temperature equilibration within a sphere:

$$\tau_{equil} = R^2 / D$$

where *R* is the radius,
and *D* is the thermal diffusivity

- Time to melt a sphere:

$$\tau_{melt} = H_m R / AI$$

where H_m is the melting enthalpy,
α is the absorptivity,
and *I* is the laser intensity

- The ordering $\tau_{equil} >> \tau_{melt}$ is typical for the Concept Laser machine
  - Powder particles are partially melted
  - Melt spreads via wetting and capillary forces
  - Un-melted particles produce porosity and weak bonding
- In the opposite case, the distribution of absorbed energy is unimportant

Conclusions

- **We have calculated the absorptivity of metal powders utilized in additive manufacturing, taking into account Fresnel reflections and multiple scattering.**
- **The absorptivity can be calculated for powders of different metals, composition, and thicknesses.**
- **The specific laser spot size can cause spatial variation of deposited energy along the beam path.**
- **Non-uniform absorption affects the dynamics of the powder melt.**